

Chloropicrin

76-06-2 | DTXSID0020315

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 61.7 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.64e-01

Confidence level: 8.37e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Chloropicrin</div> <div>Measured: 61.7</div> <div>Predicted: 61.7</div>	<div>Image not found</div> <div>1,2-Dibromoethane</div> <div>Measured: 51.3</div> <div>Predicted: 55.8</div>	<div>Image not found</div> <div>Chloroform</div> <div>Measured: 39.8</div> <div>Predicted: 50.3</div>
<div>Image not found</div> <div>Trichloroethylene</div> <div>Measured: 100</div> <div>Predicted: 83.1</div>	<div>Image not found</div> <div>1,1,2,2-Tetrachloroethane</div> <div>Measured: 79.4</div> <div>Predicted: 77.8</div>	